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GEOLOGICAL SURVEY

HEWLETT PACKARD 9845A COMPUTER PROGRAM TO
INVERT COMPLEX RESISTIVITY DATA

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Table 1--List of symbols

$Z(\omega)$	-Cole-Cole impedance
$\omega = 2\pi f$	-angular frequency
$i = \sqrt{-1}$	-imaginary number
N	-number of data points
M	-number of dispersions
n	-number of parameters
$v = N - n - 1$	-degrees of freedom
p_j	-Cole-Cole parameter ($j = 1, M * n$)
R_o	-DC resistance or apparent resistivity
m_j	-chargeability
τ_j	-time constant
c_j	-frequency dependence
x_i	-measured sampling point ($i = 1, N$)
y_i	-measured value
\hat{y}_i	-mean measurement
$y(x_i)$	-calculated value
$A_{ij} = \partial y_i / \partial p_j$	-derivative matrix
$\alpha = A^T A$	-curvature matrix
$\Delta p, \Delta p_j$	-incremental parameter change
$\bar{d} = y_i - y(x_i)$	-difference vector
I	-identity matrix
λ	-stabilization factor
w_i	-weighting factor
s^2	-functional variance

σ_i	-sample variance
σ_j	-parameter variance
χ^2_v	-reduced chi-square
$\text{cov}(p_{jk})$	-covariance matrix ($j, k = 1, M \times n$)
$\text{cor}(p_{jk})$	-correlation matrix
*	-multiplication

Introduction

This report describes an interactive Hewlett Packard (HP) 9845A computer program that inverts spectral induced polarization (SIP) or complex resistivity (CR) data. A complex (that is, frequency dependent) impedance is defined in terms of a multiplicative Cole-Cole model (Cole and Cole, 1941; Pelton, 1977; Washburne, 1982). Either amplitude, phase or amplitude-phase data can be inverted. This program utilizes Marquardt's (1963) maximum neighborhood method to stabilize the inverted derivative matrix. The reduced chi-square (Bevington, 1969) determines convergence. Both 'normal' and reversed (or 'negative') dispersions can be modeled. This allows first-order EM coupling effects to be removed from field data. Program operation is demonstrated using a calculated dispersion.

Below, SIP measurements, Cole-Cole models and inversion techniques are introduced briefly. Relevant computational procedures are reviewed in three sections under "Program description": 1) input, 2) calculations and 3) output. After noting a few program limitations, user-orientated procedural guidelines, program notes and program input/output (I/O) are reviewed.

An SIP measurement consists of recording a complex impedance (usually resolved into amplitude-phase or real-imaginary components) across a wide frequency range (.01-1000 Hz, for instance). The objective of a SIP measurement is to quantify charge polarization effects that are induced in the earth by an alternating electric field. In most rocks, this polarization can be characterized by a simple dispersion or by several dispersions. Specific mechanisms or polarizable sources cannot be attributed to these dispersions, however, because a wide range of mechanisms and overlap of active zones exist among several possible sources. Until more of the physical processes governing natural rock polarization are understood, Cole-Cole parameterization is limited to simply quantifying the spectrum of a given measurement.

Cole-Cole parameters can be defined in terms of a simple equivalent circuit (fig. 1a) or related to a hypothetical rock pore system (fig. 1b). More realistic situations consisting of a random network of these basic components also can be expressed in terms of a simple distributed circuit (Zonge, 1972). It is important to realize, however, that this solution is not unique in two

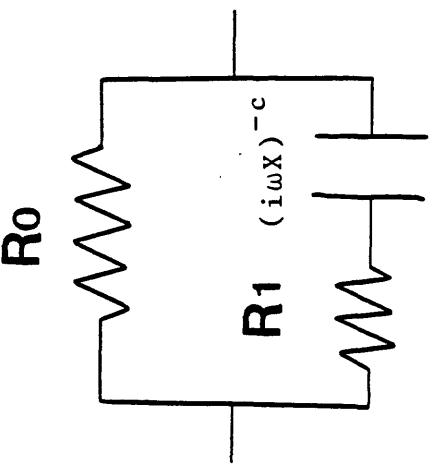


Figure 1a—Cole-Cole equivalent circuit model. The Cole-Cole parameters (R_0, m, τ, c) can be expressed in terms of a lossy circuit's impedance.

$$Z(\omega) = R_0 \left(1 - m \left(1 - \frac{1}{1 + (i\omega\tau)^c} \right) \right)$$

$$m = \frac{R_0}{R_0 + R_1} \quad \tau = \chi(R_0 + R_1)^{1/c}$$

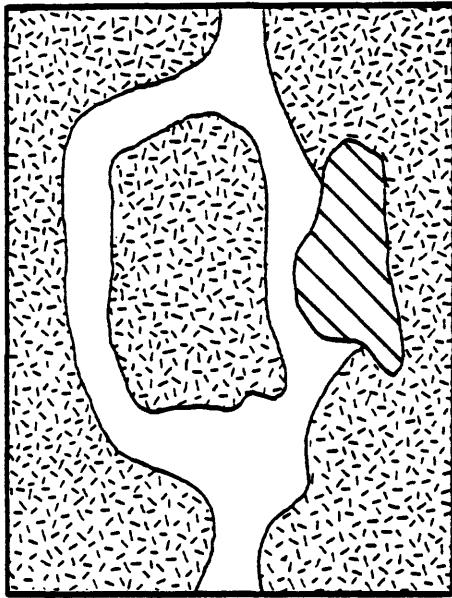


Figure 1b—A possible rock pore system approximating the equivalent circuit on the left. Two possible electrolytic paths are open; the path below interacts with a polarizable particle (diagonal shading).

important respects: 1) the Cole-Cole model is only one of many possible mathematical representations and 2) inversion of Cole-Cole models involves a linearization of a nonlinear problem. Model parameters derived from noisy data are particularly nonunique. In general, an estimate of the parameters' nonuniqueness can be obtained by carefully examining the inversion's output, which usually includes: 1) statistical measures, such as parameter standard deviation and correlation matrix and 2) intermediate parameterizations (large fluctuations are a sign of poor resolution).

Program description: Input

The program requires as input sets of frequency (Hz), amplitude ($\text{ohm}\cdot\text{m}$) and phase (mrad) measurements in order of ascending frequency. Subroutine Test (line 6130) demonstrates how the data arrays are filled. Four methods of interactively weighting the data are possible (see "Program operation"). Amplitude data are scaled using a simple logarithmic transformation; phase data are scaled using a hyperbolic sine transformation. The second transformation scales small ($-1 < x < 1$ mrad) phases linearly while larger positive and negative phases are scaled logarithmically.

Initial Cole-Cole parameters (m , τ and c) must be supplied interactively. Several families of curves (fig. 2) demonstrate the effect each parameter has on a dispersion's shape. Any parameter can be held constant to constrain the final solution. A logarithmic transformation of τ effectively limits its range to between 4 and -7. The ranges of m and c are physically constrained between 0 and 1 by the equivalent circuit representation of a Cole-Cole dispersion (Pelton et al., 1978). Constraining these two parameters with a simple trigonometric or hyperbolic transformation is ineffective because poorly resolvable parameters become fixed at unrealistic values. Therefore, it is best that these parameters be fixed as the need arises. Both m and c must be positive. Occasionally, a modified parameter becomes negative (it is displayed as a negative); however, its absolute value is used for subsequent calculations.

A weakness of the Cole-Cole model is the high inherent correlation between parameters. This is illustrated by inverting the systematically varying spectra in figure 2 and graphically summarizing the resulting parameter correlations (fig. 3). These results indicate that parametric ambiguity is greater when a dispersion is: strong (m), incomplete (τ) and/or broad (c).

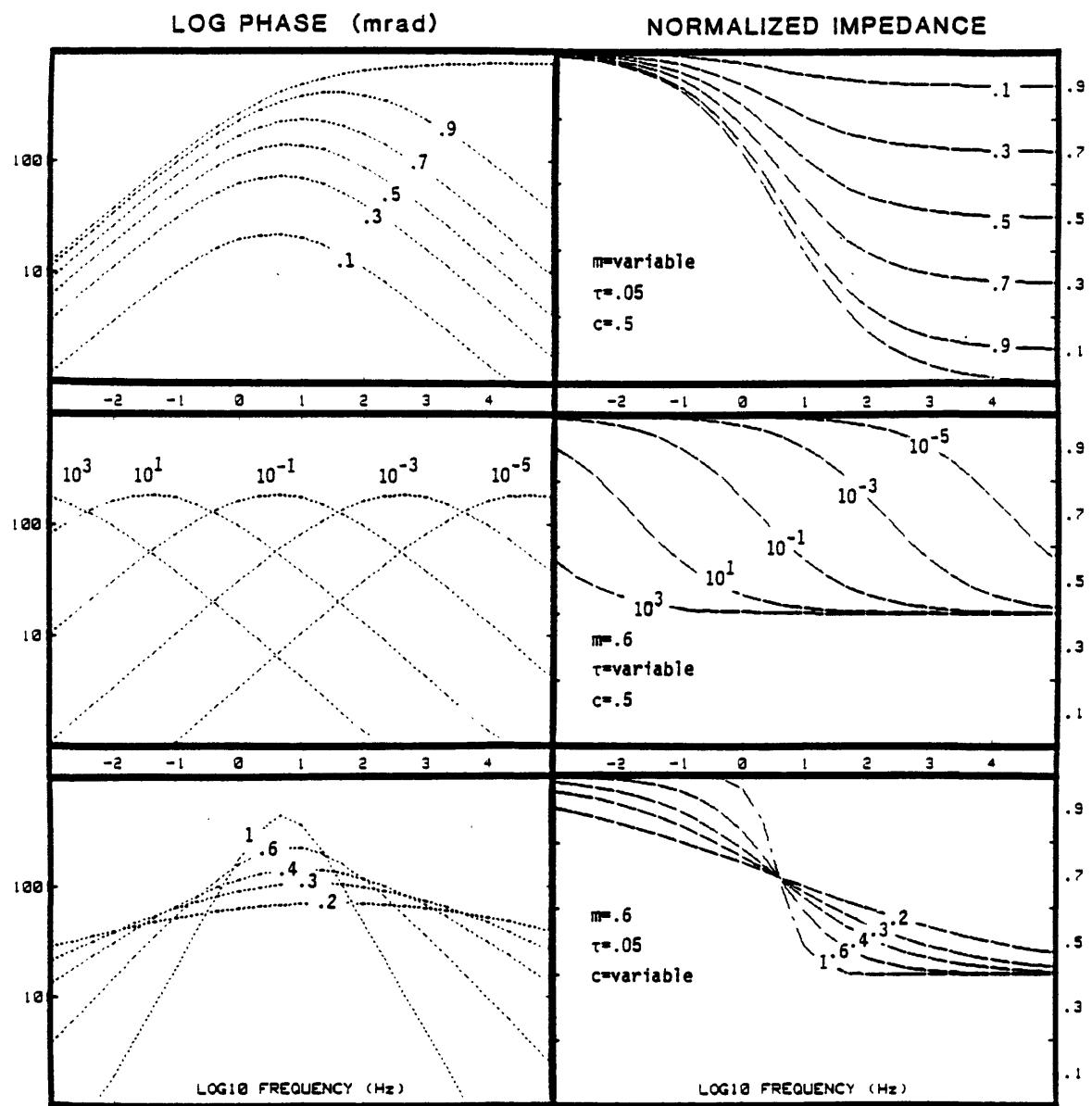


Figure 2--The effect of parametric variations on a single Cole-Cole model. Each family of curves was generated by holding two parameters constant and letting the third vary as indicated.

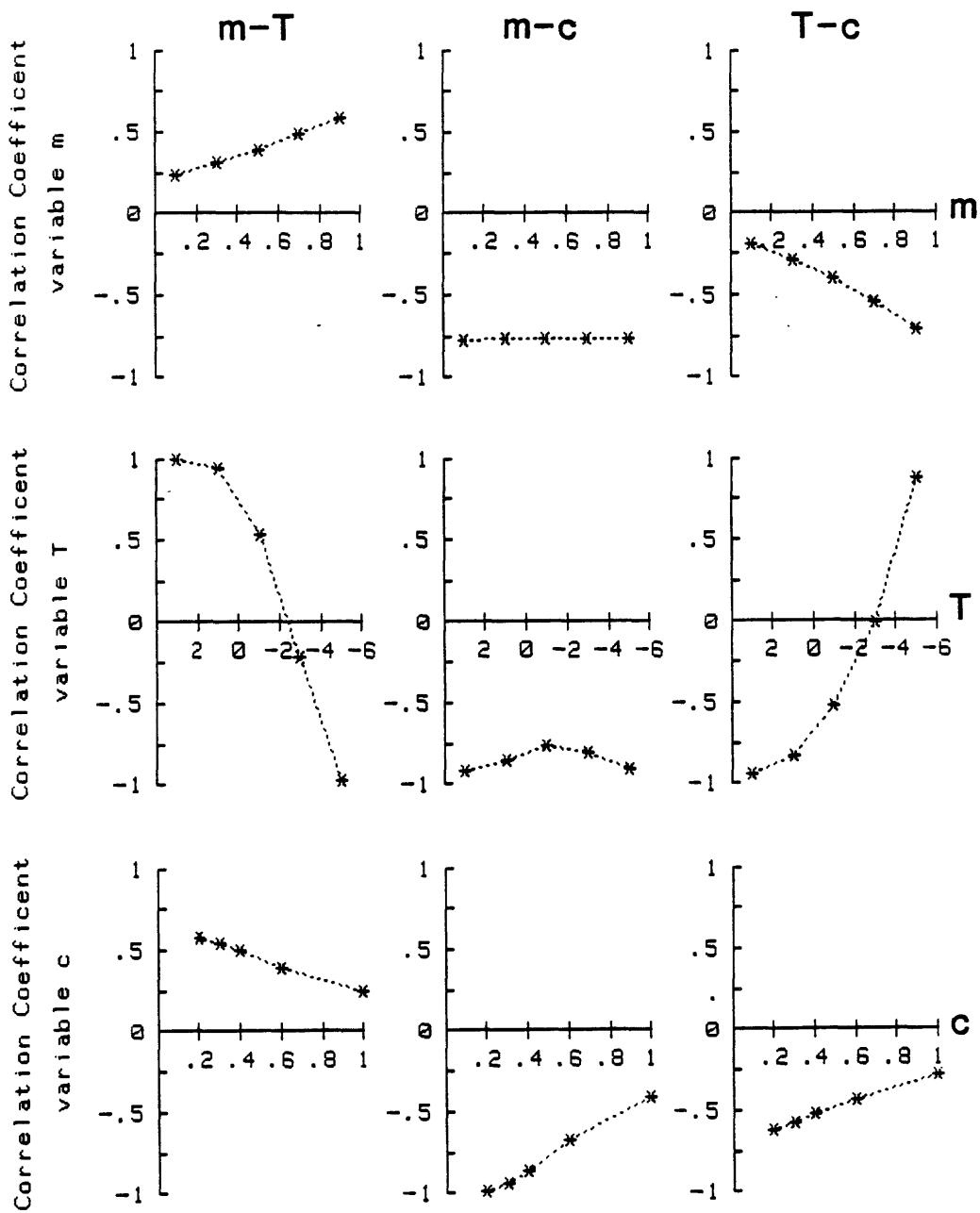


Figure 3--Cole-Cole model parameter correlations. Each dispersion in figure 2 has been inverted to form a measure of inherent parameter correlation. Constant parameters are $\eta, \tau, c = .6, .05, .5$. Variable parameters are plotted along the horizontal axis.

Program description: Calculations

The forward solution (subroutine Colem) is expressed in terms of the real and imaginary parts of a complex impedance (equations 1-2), which is modeled by a product of Cole-Cole dispersions (equation 3) (B.D. Smith, pers.commun., 1981; Washburne, 1982).

$$Z_{\text{real}} = \frac{1 - \frac{m}{D_1} (a + (\omega\tau)^2 c)}{1 + 2a + (\omega\tau)^2 c} \quad (1)$$

$$Z_{\text{imag}} = -\frac{m}{D_1} b \quad (2)$$

$$Z(\omega) = R_0 (1 - m_1 f_1)(1 - m_2 f_2) \quad (3)$$

where $a = (\omega\tau)^c \cos(c\pi/2)$

$$b = (\omega\tau)^c \sin(c\pi/2)$$

$$D_1 = 1 + 2a + (\omega\tau)^2 c$$

$$f = \left(1 - \frac{1}{1 + (i\omega\tau)^c} \right)$$

(see table 1 for a definition of these and other variables). This parameterization is useful to quantify many spectral curves simply for more detailed interpretational analysis.

The inversion subroutine (Curfit) searches a $n \times n$ parameter space for a minimum reduced chi-square between the weighted raw and inverted data points (Bevington, 1969). The impedance function is linearized by considering only the first two terms in its Taylor-series expansion (equation 4), where $Z(\omega)/R_0$ has been transformed to $y(x)$ for simplicity.

$$y_i = y(x_i) + \partial y_i / \partial p_j \Delta p_j \quad (4)$$

In matrix notation this becomes (equation 5):

$$\bar{d} = A \Delta p \quad (5)$$

Multiplying each side by A^T gives (equation 6):

$$A^T \bar{d} = A^T A \Delta p \quad (6)$$

A Marquardt-like stabilization factor (λ) is added to the main diagonal of the curvature or normalized derivative

A Marquardt-like stabilization factor (λ) is added to the main diagonal of the curvature or normalized derivative matrix to keep it from becoming singular (Marquardt, 1963). This equation can now be solved for Δp (equation 7).

$$\Delta p = (A^T A + \lambda I)^{-1} A^T \bar{d} \quad (7)$$

At each iteration, λ is changed. Initially, and away from the zone of convergence, λ is large and increasing-- the search approximating the gradient method. As a minimum is approached, however, λ is decreased and the search approximates the linearized expansion method, which converges quadratically in this region. Convergence is reached when either the incremental or relative chi-square error becomes less than some tolerance. The tolerance defaults to 10^{-4} for phase and amplitude-phase inversion options and to 10^{-5} for the inversion of amplitude. These might need to be modified for exceedingly good or noisy data sets. Because these tolerances are derived from experience with theoretical, laboratory and field data sets, it appears as though the inversion of logarithmic amplitude data is less sensitive to parametric variations than is the inversion of logarithmic phase data.

Either numeric or analytic derivatives can be used in this program. The only significant difference between the two methods is the much greater speed at which analytic derivatives are calculated; the time savings is a function of the number and resolvability of the parameters. Numerical derivatives are calculated by perturbing each parameter, in turn, by 10% and finding the differential: $\Delta y / \Delta x$. Analytic derivatives are derived from the partial derivatives (equations 8-10) of a single Cole-Cole dispersion.

$$\frac{\partial y}{\partial m} = 1/D_1 [a + (\omega\tau)^{2c} - i b] \quad (8)$$

$$\frac{\partial y}{\partial \tau} = mc/(D_1\tau) [R + I] \quad (9)$$

$$\frac{\partial y}{\partial c} = m/D_1^2 [R \ln(\omega\tau) - I\pi/2 + i(R\pi/2 + I \ln(\omega\tau))] \quad (10)$$

where $R = 2(\omega\tau)^{2c} + a[1+(\omega\tau)^{2c}]$

$$I = b [1-(\omega\tau)^{2c}].$$

Since amplitude and phase are defined as (equations 11-12),

$$A = \sqrt{Z_{\text{real}}^2 + Z_{\text{imag}}^2} \quad (11)$$

$$\phi = \tan(Z_{\text{imag}}/Z_{\text{real}}), \quad (12)$$

analytic derivatives have the form of equations 13-14:

$$\frac{\partial A}{\partial p} = \frac{1}{A} \left(\frac{\partial Z_{\text{real}}}{\partial p} + \frac{Z_{\text{imag}}}{Z_{\text{real}}} \frac{\partial Z_{\text{imag}}}{\partial p} \right) \quad (13)$$

$$\frac{\partial \phi}{\partial p} = \frac{1}{A^2} \left(\frac{\partial Z_{\text{imag}}}{\partial p} - \frac{Z_{\text{imag}}}{Z_{\text{real}}} \frac{\partial Z_{\text{real}}}{\partial p} \right). \quad (14)$$

Pelton et al. (1978) note that a Cole-Cole model whose frequency dependence is one can be used to decouple 'normal' high frequency EM coupling effects from lower frequency IP effects. Although parametric resolution is lost (Major and Silic, 1980) and this procedure is valid only before the phase maximum in simple geoelectric environments (Webster, 1980), it is a useful first approximation. 'Negative' coupling effects can be removed in a like manner by using two opposing Cole-Cole dispersions to model the coupling (Hallop and Pelton, 1980) (equations 15-16).

$$Z(\omega) = R_0 (1 - m_1 f_1) (1 - m_2 f_2) \quad (15)$$

$$Z(\omega) = R_0 (1 - m_1 f_1) (1 - m_2 f_2) (1 + m_3 f_3) \quad (16)$$

----- coupling -----

Residual phases are calculated by decomposing the modeled real and imaginary parts of the spectrum from the real and imaginary (that is, cosine, sine) representation of the original spectrum.

Program description: Output

The program outputs: 1) inverted Cole-Cole parameters, 2) several statistical measures of the inversion's fit and the parameter's ambiguity and 3) a plot of the raw and inverted dispersions.

There are several measures of "goodness of fit". Bevington (1969) defines the functional variance (s^2) of a set of data (y_i) to a fitting function ($y(x_i)$) as (equation 17):

$$s^2 = 1/v \sum_i w_i [y_i - y(x_i)]^2 \quad (17)$$

where the weighting function, w_i (equation 18), is normalized in terms of the sample variances, σ_i (equation 19).

$$w_i = \frac{1/\sigma_i^2}{1/N \sum_i 1/\sigma_i^2} \quad (18)$$

$$\sigma_i = \frac{1}{N} \sum_i (y_i - \hat{y}_i)^2 \quad (19)$$

The reduced chi-square (χ_v^2) (equation 20) is a measure of how well a fitting function matches a series of observations and is found by taking the ratio of the functional variance to the weighted average of the sample variances ($\sigma_i^2 = w_i \sigma_i^2$).

$$\chi_v^2 = 1/v \sum_i [y_i - y(x_i)]^2 = s^2 / \bar{\sigma}_i^2 \quad (20)$$

Ideally, the reduced chi-square is unity-- larger values indicating a poor fit, smaller values indicating a larger uncertainty in the observations. If sample variance is unknown, $\sigma_i^2 = 1$, and the reduced chi-square is simply the least-squares error.

Parameter error can be estimated from the covariance matrix (equation 21).

$$\text{cov}(p_{jk}) = [A^T A]^{-1} \chi_v^2 \quad (21)$$

Diagonal elements of $\text{cov}(p_{jk})$ indicate parameter variance (σ_j), non-diagonal elements indicate parameter covariance. For reasonable parameterizations, the normalized covariance or correlation matrix (equation 22) gives a measure of the correlation between parameters.

$$\text{cor}(p_{jk}) = \frac{\text{cov } p_{jk}}{\sqrt{\text{cov } p_{jj} \text{cov } p_{kk}}} \quad (22)$$

A correlation of zero indicates an independent parameter. Coefficients of +1 and -1 indicate a strong correlation or inverse correlation, respectively.

Following the statistics, raw and inverted dispersions are plotted. A plot of logarithmic phase lag and normalized (by R_o) amplitude versus logarithmic frequency is preferred because Cole-Cole parameters are estimated easily from this presentation. Data can be plotted on a normalized real-imaginary axis diagram (also known as an Argand or Cole-Cole diagram). For the benefit of those who prefer this format, the raw data are plotted on a reduced real-imaginary diagram also.

Program limitations

When comparing this data to other Cole-Cole modeled data, beware of slight but parametrically significant differences in the way multiple dispersions are defined.

Three dispersion models are adequate to fit most laboratory and field SIP data. If more complicated models are desired, the 9845A's 64K byte memory must be extended or advantage taken of overlapped processing.

The validity of inversion statistics depends upon:
1) spectral resolvability in terms of the Cole-Cole model
and 2) linearity of the Taylor-series approximation. At best, statistics serve only as relative indications of parametric stability and correlation.

The Cole-Cole model only approximates EM coupling. As a result, parameters associated with high frequency polarization dispersions are ambiguous. In general, however, this is a good enough approximation so that parameters associated with low frequency dispersions are more characteristic of a coupling-free environment.

Procedural Guidelines

- 1) Weight to 0 those points that are not part of a smooth spectral curve. One 'bad' point, especially at a frequency extreme, can wreck convergence.
- 2) Determine how many polarization dispersions are present. Be sure to note models that do not truly correspond to a single dispersion (that is, where impulsive or transitory behavior is not fit well by a simpler model). Minimize the number of models.
- 3) Initialize the model. Hold unresolvable parameters constant. Refer to Figure 2 if you have difficulty relating spectral shape to the Cole-Cole parameters. In general, resolvable parameters are characterized by: 1) clear non-zero slopes (>4 pts) and 2) clearly distinguishable phase peaks (>50 mrad); unresolvable parameters are characterized by: 1) very low slopes and phase peaks (m, τ, c) and 2) phase maxima outside the measuring range (m, τ). First, minimize the number of constant parameters. Later, use insight gained from a set of spectra to determine which of the most ambiguous parameters to hold constant.
- 4) There will always be a better fitting model. When the data is fit adequately, stop inverting and start interpreting!

General Program Conventions and Notes

SYSTEM: Hewlett Packard (HP) 9845A/ 64K byte memory. Refer questions regarding HP BASIC syntax to the HP 9845 manuals: "Operating and programing" and "Graphics programing techniques".

UNITS: Unless otherwise noted, assume the following units: meters, milliradians, ohm-meters, volts, amperes.

DEFAULTS: All questions have default values preassigned. Pushing CONT (continue) executes these defaults. The default response is indicated by underlining.

VARIABLES: Variable names are usually mnemonics related to their function. In general, a given variable's definition is ubiquitous to the whole program. This program's most important variables are defined in table 2.

PROGRAM HEADERS: Definitions of parameters passed to each subroutine are found in its heading. Array dimensions are indicated in parenthesis. Descriptive line labels provide access to the head of each subroutine if this is required.

USER MODIFICATIONS: There are a few places where the user might want to set a default variable in the program. A few of the most likely modifications are described below.

Begin by pushing EDITLINE ...; finish by pushing STORE.

1) The internal printer is activated by changing the device code, Pdev, in line 390 from 16 to 0. Activating lines 2100 and 2250 will keep intermediate parameters from being printed out when Pdev=0.

2) A double logarithmic phase scale (to plot both positive and negative phases) is activated by changing the variable Log\$ in line 400 from "YES" to "DBL".

3) Numeric, rather than analytic derivatives, will be calculated if the variable Analytics\$ in line 1080 is changed from "YES" to "NO".

4) The default input device variable Device\$ can be changed in line 6240 from ":C" (disk) to ":T14" (left-hand tape drive), for instance.

5) The log-log plot's base and frequency range are easily modified in lines 750 and 5300. These default to: $\text{base}=10$, $f_{\min}=-3$ and $f_{\max}=5$. Either plot can be suppressed by deactivating (with $W!#$) the appropriate line (see lines 750, 770, 5300 or 5310). Note that if subroutine Crplt is not called before Argplt, the plotter must be initialized. Change line 8910 to: PLOTTER IS 13, "GRAPHICS"-- to accomplish this.

6) Occasionally, weak dispersions are incorrectly scaled in the final plot. This condition exists when a large DC offset is obvious between the raw and inverted normalized amplitudes. To replot the data correctly, temporarily modify Rk in line 7070 from 1 to R0.

Table 2--List of major variables

Below, the most important common, passed and calculated variables or arrays are defined. Default values are indicated in parentheses.

```
I=1,Nf
J=1      -raw data
        =1+x   -model x           if model=1
        =2+model -inverted data   then J=2 -inverted
        =3+model -residual
K=1,2*Nf
        1st half: amplitudes;   2nd half: phases
```

COMMON:

```
Nf -number of frequencies                               (41)
model -number of Cole-Cole dispersions modeled      (2)
R0 -DC apparent resistivity; initially set to Amp(1,1)
F(I,I)          -frequency
Amp(J,I)        -amplitude
Phz(J,I)        -phase
Constant(*)     -constant parameters             (1)
                l=variable; 0=constant
```

PASSED:

```
Y(I,K)          -input or raw data
Yfit(I,K)       -output or best fit
Sigy(I,K)       -standard deviations
Ywt(I,K)        -data weights                  (1)
P(3,model)      Cole-Cole parameters
```

CALCULATED:

```
A(I,model*3)    Derivative matrix
Dp(model*3,model*3) Inverted incremental parameters
```

User Instructions: Program I/O

The following example uses the theoretically-calculated response of two RC circuits in series. Both circuits have a Warburg-like ($\sim\sqrt{f}$) capacitance. Below, a typical program run (listed in appendix A) is broken-down into 16 steps. System commands are capitalized. Commonly occurring program variables are offset by a double hyphen (--X).

- A. Turn on the machine and insert the program tape into the right-hand (T-15) tape drive. Insert the data tape into the left-hand (T-14) tape drive.
- B. Type GET "CRDBL", and press EXECUTE.
- C. When the program is loaded, press RUN. Several prompting statements will appear successively on the screen and the user should type the appropriate responses as follows:
 - 1) Today's date? (Mo/Da/Yr) End by pressing CONT. --Date\$
 - 2) Read from? : --Iofile\$
Choose the proper subroutine to read in the data, CONT.
 - 3) File name? : Enter the data file name, CONT. --Fnm\$
 - 4) Do you want to PLOT or ... CONT? : This allows the data to be previewed for the purpose of weighting points and choosing the initial inversion model. After generating the plot, the program waits three seconds and will continue automatically unless PAUSE is executed.
 - 5) What do you want to invert? Type one number, CONT. --Iop
 - 6) Choose one method of weighting the data? Four modes are possible:

Mode 1: Instrumental- use when measurement standard deviations are known.

Mode 2: Statistical- assumes a statistical relationship where errors are proportional to magnitude.

Mode 3: Selective- allows arbitrary weights to be assigned to each data point. In turn, amplitude and phase data are displayed, five points per line. A row of "1"'s, also offset in groups of five, will be displayed at the bottom of the screen. These are default weights. Use the <-- and --> keys to position the cursor under the data

point that is to be reweighted. CONT when finished.

Mode 4: None- assigns equal weights of "1" to each data point (default).

- 7) At this point, a tabulated summary of the data is printed to the device specified by Pdev (line 390). In this example, frequency (Hz), amplitude (ohm-m) and phase (mrad) are printed with their respective weights. Note that these are values of phase shift whereas phase lag is plotted.
- 8) How many dispersions ... do you want to model? --model
Refer to "Procedures". End with CONT.
- 9) Input M,T,C: --P(*)
Requests initial Cole-Cole parameters, CONT.
- 10) Are these correct? : Requests confirmation that parameters have been entered correctly. Typing NO branches back to step 9. CONT.
- 11) Do you want to hold one parameter constant?: Allows one parameter of current model to be held invariant during inversion. CONT.
- 12) "Which one?:" Requests parameter to be held constant. This loop must be passed through for each parameter held constant. CONT.

At this point, the computer starts inverting the data. If, for any reason, the inversion is terminated prematurely by pushing special function key "k8" (ie. wildly fluctuating or unrealistic parameters), the program should jump to step 13 (ie, statistics will be calculated for the last iteration). Unfortunately, if k8 is pushed during an intermediate calculation, the statistics and inverted plot might be invalid. Avoid this situation by pushing k8 immediately following the display of an intermediate result.

- 13) Intermediate results are printed on the device specified by Pdev following each iteration. This output consists of:

- a) Fixed parameters, if any.
- b) Free Cole-Cole parameters for each iteration. The column headings are:

It: iteration -iteration 0 lists initial parameters.
Lamda(λ): Marquardt stabilization factor.

Rchisqr: Reduced chi-square.

M,T,C: Cole-Cole parameters m, τ and c.

c) %Sigma= parameter standard deviations.

d) Correlation matrix. If inversion option (Iop) 1 or 3 was chosen (amplitude or both, respectively), an additional parameter (DC resistivity) is used to find parameter correlations. Its relationship to other parameters is found in the matrix's last row.

14) Type YES to plot your results. Type NO to change parameters, CONT. Program loops back to step 8 if this parameterization is not satisfactory. For the novice using this program, 'bad' data points are the cause of poor parameterizations more often than are unresolvable dispersions. If this is the case, start over from the beginning by pushing STOP twice and then RUN.

15) Which dispersion do you want to remove? Enter the dispersion or model number, CONT. This step is skipped if 0 is typed.

16) The final plot is automatically displayed on the screen. Type DUMP GRAPHICS and press EXECUTE, to get a hard copy.

WHAT IS PLOTTED:

Normalized amplitude (Z/R_o) (0)

Inverted amplitude - - - - -

Log₁₀ phase lag (+ or - ; # if $w_i=0$)

Inverted dispersions -----

Residual phase - - - - -

$R_{dc}=R_o$: Calculated zero frequency apparent resistivity

A real-imaginary axis diagram of the data is made in the lower left-hand corner. Each curve is normalized by R_o . The axes are negative upwards and to the left and are graduated at 10% increments and labeled every .5 units. Only the inverted dispersion is plotted (see USER MODIFICATIONS). Points weighted to zero are skipped. Plus (+) symbols mark every fourth frequency point.

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Appendix A
Example Program Listing

The following listing was made by assigning PRINT ALL IS 0 and depressing the PRINT ALL key. Each step is described in the User Instructions section of this report. Under normal operating conditions, only the two output sections indicated by a double line in the right-hand margin will be output to the thermal printer when Pdev=0.

- 1) Enter todays date(m/d/y):
1/31/82
- 2) Read data from TEST, In1, or In2?
TEST
- 3) TEST:Filename?
mRCser
- 4) Do you want to PLOT and preview the spectrum or CONT?
PLOT

1) Just Amplitude

2) Just Phase

3) Both Amp and Phz

- 5) What do you want to invert?
3

1) Instrumental (1/sig^2)

2) Statistical (1/Y)

3) Selective (1-0)

4) None (1)

- 6) Choose one method of weighting the data?
3

AMPLITUDE

1.97E+00	1.95E+00	1.91E+00	1.85E+00	1.77E+00
1.68E+00	1.60E+00	1.54E+00	1.49E+00	1.43E+00
1.36E+00	1.28E+00	1.19E+00	1.12E+00	1.07E+00
1.04E+00	1.02E+00			

Edit the weighting function; then CONT.

1, 1, 1, 1, 1| 1, 1, 1, 1, 1| 1, 1, 1, 1, 1| 1, 1

PHASE

-1.41E+01	-2.31E+01	-3.57E+01	-5.01E+01	-6.14E+01
-6.41E+01	-5.91E+01	-5.33E+01	-5.35E+01	-6.18E+01
-7.54E+01	-8.63E+01	-8.51E+01	-7.08E+01	-5.10E+01
-3.32E+01	-2.03E+01			

Edit the weighting function; then CONT.

1, 1, 1, 1, 1| 1, 0, 1, 1, 1| 1, 1, 1, 1, 1| 1, 1

13) CONSTANT PARAMETERS: C1: 5.00E-01

<u>It</u>	<u>Lamda</u>	<u>Rchisq</u>	<u>M1</u>	<u>T1</u>	<u>M2</u>	<u>T2</u>	<u>C2</u>
0	0E+00	3.96E-01	5.00E-01	1.00E+00	5.00E-01	1.00E-03	3.00E-01
1	1E-01	1.03E-02	2.25E-01	9.55E-01	3.32E-01	5.99E-04	4.35E-01
2	1E-02	2.52E-04	2.50E-01	1.24E+00	3.30E-01	3.69E-04	4.99E-01
3	1E-03	4.41E-08	2.48E-01	1.20E+00	3.35E-01	4.00E-04	5.00E-01

%Sigma= 3.86E-02 3.19E-02 3.20E-02 3.77E-02 2.92E-02

CORRELATION MATRIX

1	1.000						
2	-.732	1.000					
3	-.650	.588	1.000				
4	-.710	.616	.714	1.000			
5	.587	-.451	-.588	-.677	1.000		
6	.219	-.071	.038	-.009	.057	1.000	

The reduced chi square has converged or diverged.

Type YES to plot your results. Type NO to change parameters.

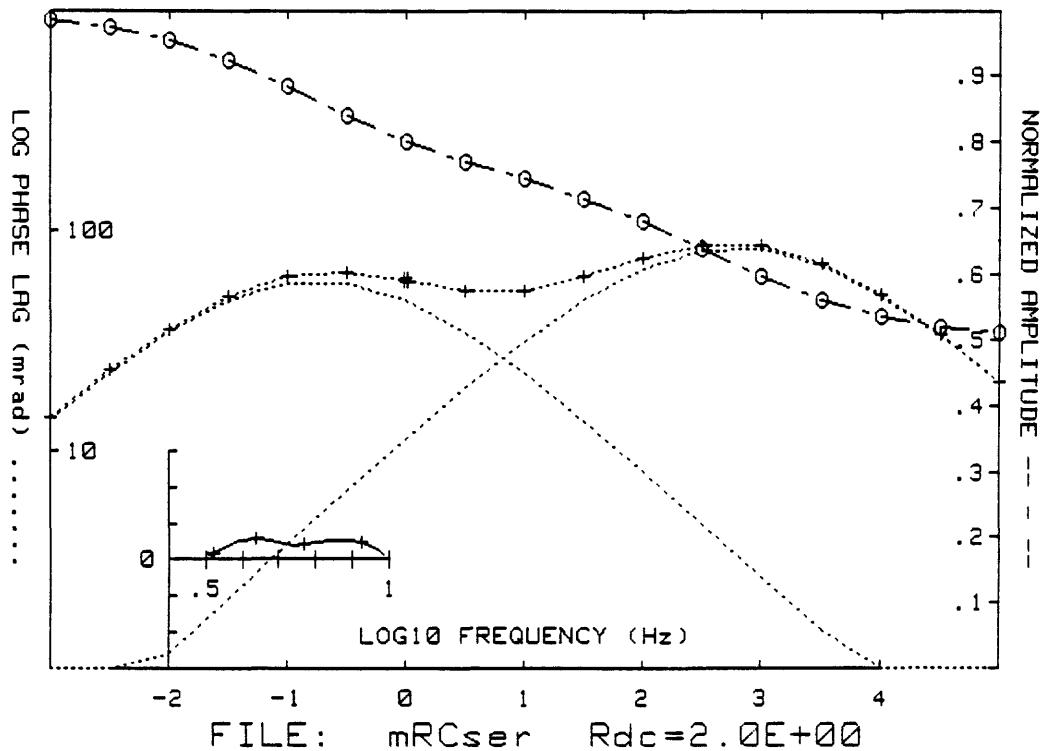
14) PLOT?

YES

Which dispersion do you want to remove(0,1,2,3)?

15) 0

16) DUMP GRAPHICS



Appendix B
Source Program Listing

```

10 ! ****
20 !
30 ! PROGRAM "CRIDBL": SPECTRAL IP INVERSION AND PLOTTING
40 !
50 ! SYSTEM: HP 9845A
60 ! AUTHOR: JIM WASHBURN
70 ! ADDRESS: U.S. DEPARTMENT OF THE INTERIOR
80 ! GEOLOGICAL SURVEY
90 ! MAIL STOP 964
100 ! BOX 25046, DENVER FEDERAL CENTER
110 ! DENVER, CO 80225
120 ! LAST REVISION: 1/31/82
130 !
140 ! SUBROUTINE ACCESS ADDRESSES:
150 ! Crinv      10- 790
160 ! Curfit     800-4000
170 !          (Dy,Norm,Output)
180 ! Colem      4010-5070
190 ! Weight     5080-6120
200 ! Readin     6130-6520
210 !          (Test,In1,In2)
220 ! Crplt      6530-7290
230 ! Plots      7300-8450
240 !          (Rescale,Linplt,Xax1bl,Yax1bl,Title)
250 ! Argplt     8460-9210
260 ! ****
270 Crinv!:!
280 OPTION BASE 1
290 COM Nf,Model,Pdev,Iop,Log$(3),Fnm$(6),Date$(8)
300 COM SHORT R0,F(1,41),Amp(6,41),Phz(6,41),Constant(3,3)
310 SHORT Y(1,82),Yfit(1,82),Sigy(1,82),Ywt(1,82)
320 DEFAULT ON                                     !SUPPRESS NON-FATAL ERRORS
330 EXIT GRAPHICS
340 PRINTER IS 16
350 PRINT PAGE
360 MAT Amp=ZER
370 MAT Phz=ZER
380 MAT Constant=ZER
390 Pdev=16                                         !PRINTER(16 or 0)
400 Log$="YES"                                       !ABSOLUTE OR DOUBLE LOG SCALE
410 INPUT "Enter todays date(m/d/y):",Date$ !("YES" or "DBL")
420 Iofile$="TEST"
430 Read: INPUT "Read data from TEST, In1, or In2?",Iofile$
440 IF Iofile$="TEST" THEN CALL Test(Y(*),Sigy(*),Ywt(*))
450 !      * * *                                * * *
460 !      * * * User supplied input programs * * *
470 !      * * *                                * * *
480 Nf2=Nf*2
490 REDIM F(1,Nf),Y(1,Nf2),Yfit(1,Nf2),Sigy(1,Nf2),Ywt(1,Nf2)
500 Invert: CALL Curfit(Nf2,F(*),Y(*),Ywt(*),Yfit(*))
510 IF Model=1 THEN Plot
520 Decupl: Decupl$="N"

```

```

530 Ans=0
540 INPUT "Which dispersion do you want to remove(0,1,2,3)?",Ans
550 IF Ans=0 THEN Plot
560 Decup1$="Y"
570 M=Ans+1
580 Rk=1
590 IF (Amp(M,1)>1.5) OR (Amp(M,1)<.5) THEN Rk=R0
600 Last=Model+3
610 FOR I=1 TO Nf
620     Ro=Amp(1,I)/R0*COS(Phz(1,I)/1000)
630     Io=Amp(1,I)/R0*SIN(Phz(1,I)/1000)
640     Re=Amp(M,I)/Rk*COS(Phz(M,I)/1000)
650     Im=Amp(M,I)/Rk*SIN(Phz(M,I)/1000)
660     R2=1-Re                         !RESIDUALS
670     I2=-Im
680     Dr=I2^2+(1-R2)^2
690     Rr=(Ro*(1-R2)-Io*I2)/Dr
700     Ir=(Ro*I2+Io*(1-R2))/Dr
710     Amp>Last,I)=R0*SQR(Rr^2+Ir^2)
720     Phz>Last,I)=1000*ATN(Ir/Rr)
730 NEXT I
740 !
750 Plot: CALL Crplt(10,-3,5,Decup1$,Ywt(*))
760 !
770 CALL Argplt(Ywt(*))
780 STOP
790 END

```

```

800 ! ****
810 !
820 Curfit!:! 11/81
830 ! A LEAST-SQUARES FIT TO A NON-LINEAR FUNCTION WITH A
840 ! LINEARIZATION OF THE FITTING FUNCTION
850 ! AFTER:P.R.BEVINGTON,1969,DATA REDUCTION AND ERROR ANALYSIS
860 !
870 !
880 SUB Curfit(Nf2,SHORT X(*),Y(*),Sigy(*),Yfit(*))
890 !
900 ! X(*): independent variable (1,Nf)           !1
910 ! Y(*): dependent variable (1,Nf2)          !2
920 ! Sigy(*): standard deviations of Y (1,Nf2)
930 ! Yfit(*): output, best fit to Y (1,Nf2)
940 !
950 OPTION BASE 1
960 COM Nf,Model,Pdev,Iop,Log$[3],Fnm$[6],Date$[8]
970 COM SHORT R0,F(*),Amp(*),Phz(*),Constant(*)
980 SHORT P(3,3),Pp(3,3),Ro
990 SHORT Dy(1,Nf2),A(Nf2,10),At(10,Nf2),W(10,Nf2)
1000 SHORT One(10,1),Beta(1,10),Dp(1,10),Sigp(1,10)
1010 SHORT Alpha(10,10),Array(10,10),Anorm(10,10),Covar(10,10),Cor(10,10),D(10,10)
1020 Initialize!:!
1030 Nterms=3
1040 Lamda=.1
1050 Iteration=1
1060 Tol=1E-4
1070 IF Iop=1 THEN Tol=1E-5 !ONLY FOR AMPLITUDE
1080 Analytic$="YES" !ANALYTIC DERIVATIVES("YES" or "NO")
1090 P4=1 !INVERT R0?(0=NO, 1=YES)
1100 IF Iop=2 THEN P4=0
1110 Conv$="NO"
1120 ! Pdev=0 !REMOVE "!" FOR LISTING OF ONLY INITIAL/FINAL PARMs
1130 PRINTER IS 16
1140 MAT Yfit=<1>
1150 MAT Constant=<1>
1160 P parms: Model=2
1170 INPUT "How many dispersions?(default:2, max:3)",Model
1180 Nparms=Nparm=Model*Nterms+P4
1190 IMAGE 3?("* ")
1200 IMAGE X,"CHARGEABILITY=",D.3D,2X,"TIME CONSTANT="D.DDE,2X,"FRE
QUENCY DEPENDENCE=",D.3D
1210 PRINT USING 1190
1220 FOR M=1 TO Model
1230     PRINT "MODEL ",M
1240     INPUT "INPUT M,T,C:",P(M,1),P(M,2),P(M,3)
1250     PRINT USING 1200;P(M,1),P(M,2),P(M,3)
1260     PRINT USING 1190
1270     Ans$="YES"
1280     INPUT "Are these correct?(YES or NO)",Ans$

```

```

1290      IF Ans$="NO" THEN 1230
1300      Ans$="NO"
1310      INPUT "Do you want to hold one parameter constant?(YES or
NO)",Ans$
1320      IF Ans$="NO" THEN 1370
1330      INPUT "Enter one parameter you want to hold constant(1,2,
or3):",J
1340      Constant(M,J)=0           !0=CONSTANT, 1=VARIABLE(default)
1350      Nparm=Nparm-1
1360      GOTO 1300
1370  NEXT M
1380  Npts=Nf
1390  IF Iop=3 THEN Npts=Nf2
1400  Nfree=Npts-Nparm
1410  IF Nfree>0 THEN Calc
1420  DISP "Degrees of freedom are zero. Program has stopped."
1430  STOP
1440  Calc: ON KEY #8 GOTO Conv
1450  DISP "Don't bother me, I'm computing . . . Press k8 to termina
te inversion"
1460  REDIM P(Model,3),Pp(Model,3)
1470  Redim:REDIM A(Nf2,Nparm),At(Nparm,Nf2),W(Nparm,Nf2)
1480  REDIM One(Nparm,1),Beta(1,Nparm),Dp(1,Nparm),Sigp(1,Nparm)
1490  REDIM Alpha(Nparm,Nparm),Array(Nparm,Nparm),Anorm(Nparm,Nparm)
1500  REDIM Covar(Nparm,Nparm),Cor(Nparm,Nparm),D(Nparm,Nparm)
1510  GOSUB Ro
1520  Ro=R0
1530  IF P4=0 THEN R0=1
1540  FOR I=1 TO Nf
1550    CALL Colem(I,1,Analytics$,Yfit(1,I),Yfit(1,I+Nf),P(*),A(*))
1560  NEXT I
1570  R0=R0
1580  GOSUB Ro
1590  Ro=R0
1600  IF P4=1 THEN R0=1
1610  GOSUB Rchisqr          !EVALUATE INITIAL ERROR
1620  R0=R0
1630  Rchisq0=Rchisq
1640  Zero:      MAT Beta=ZER          !INVERSION
1650          MAT Alpha=ZER
1660          MAT One=(1)
1670  IF Conv$="YES" THEN Beta
1680  IF Analytics$="NO" THEN GOSUB Numeric   !NUMERIC DERIVATIVES
1690  Beta:      MAT Dy=Dy.Sigy
1700          MAT Beta=Dy*A
1710  Alpha:     MAT W=One*Sigy
1720          MAT At=TRN(A)
1730          MAT At=At.W
1740          MAT Alpha=At*A
1750  Norm:      CALL Norm(Nparm,Alpha(*),Anorm(*))
1760  Stabilize: MAT D=IDN
1770          MAT D=D*(Lamda)

```

```

1780      MAT Array=Anorm+D
1790  Invert:   MAT Array=INV(Array)
1800  IF Conv$="YES" THEN Stats
1810      MAT Array=Array.Anorm
1820      MAT Array=Array/Alpha
1830      MAT Dp=Beta*Array
1840  Jm=0                                !CALCULATE NEW PARAMETERS
1850  FOR M=1 TO Model
1860    FOR J=1 TO Nterms
1870      Pp(M,J)=P(M,J)
1880      IF Constant(M,J)=0 THEN Nextj
1890      IF J=2 THEN Pp(M,J)=LGT(Pp(M,J))
1900      Jm=Jm+1
1910      Pp(M,J)=Pp(M,J)+Dp(1,Jm)
1920      IF J=2 THEN Pp(M,J)=10^Pp(M,J)
1930  Nextj:  NEXT J
1940  NEXT M
1950  R0o=R0=R0
1960  IF P4=0 THEN R0=1
1970  IF P4=1 THEN R0=R0+Dp(1,Jm+1)
1980  FOR I=1 TO Nf
1990    CALL Colem(I,1,Analytics$,Yfit(1,I),Yfit(1,I+Nf),Pp(*),R(*))
2000  NEXT I
2010  IF P4=0 THEN R0=R0
2020  IF P4=0 THEN GOSUB Ro
2030  R0=R0
2040  IF P4=1 THEN R0=1
2050  GOSUB Rchisqr                         !RE-EVALUATE ERROR
2060  R0=R0
2070  Io:IF Iteration<>1 THEN Ckerr
2080  CALL Output(0,Model,Nterms,0,0,0,0,P(*))
2090  CALL Output(1,Model,Nterms,0,0,Rchisq0,5,P(*))
2100 ! Pdev=16 REMOVE "!" FOR LISTING OF INITIAL/FINAL PARMs ONLY
2110 Ckerr:IF (ABS(Rchisq/Rchisq0)<=Tol) OR (ABS(Rchisq0-Rchisq)<=Tol) THEN Conv
2120      IF Rchisq<Tol/100 THEN Conv
2130  CALL Output(1,Model,Nterms,Iteration,Lamda,Rchisq,5,Pp(*))
2140  IF Lamda>=10000 THEN End
2150  Iteration=Iteration+1
2160  IF Rchisq0-Rchisq>=0 THEN GOTO Less
2170  More: Lamda=10*Lamda                  !ERROR HAS INCREASED
2180  IF P4=1 THEN R0=R0
2190  GOTO Stabilize
2200  Less: Lamda=Lamda/10                  !ERROR HAS DECREASED
2210  MAT P=ABS(Pp)
2220  Rchisq0=Rchisq
2230  GOTO Zero
2240  Conv: Conv$="YES"                     !ERROR HAS CONVERGED
2250 ! Pdev=0 REMOVE "!" FOR LISTING OF INITIAL/FINAL PARMs ONLY
2260  CALL Output(1,Model,Nterms,Iteration,Lamda,Rchisq,5,Pp(*))
2270  Lamda=0
2280  MAT P=Pp

```

```

2290 IF P4=1 THEN GOTO Zero
2300 M=Model+2
2310 IF Model=1 THEN M=2
2320 Ct=0
2330 Dsum=0
2340 Shift=0
2350 IF Iop=2 THEN Shift=Nf
2360 FOR I=1 TO Nf
2370   IF Sigy(1,I+Shift)=0 THEN 2400
2380   Dsum=Dsum+LOG(Amp(1,I)/Amp(M,I))
2390   Ct=Ct+1
2400 NEXT I
2410 R0=EXP(Dsum/Ct)           !AVERAGE R0 @ CONVERGENCE
2420 GOTO Zero
2430 Stats: REDIM One(1,Nparm)
2440   MAT One=(1)
2450   MAT Covar=Array*(Rchisq)
2460   MAT D=IDN
2470   MAT D=D.Covar
2480   MAT D=SQR(D)
2490   MAT Sigp=One*D
2500   MAT Sigp=Sigp*(100)
2510   CALL Norm(Nparm,Covar(*),Cor(*))
2520 CALL Output(2,Model,Nterms,0,0,0,22,Sigp(*)) !UNCERTAINTIES
2530 OUTPUT Pdev USING "18A";"CORRELATION MATRIX"
2540 CALL Output(3,Nparm,Nparm,0,0,0,19,Cor(*))
2550 GOTO End

```

```

2560 Numeric: DEF FNAsnh(SHORT X)=LOG(X+(X^2+1)^.5)
2570 SHORT Yfita,Yfitp
2580 Ro=R0
2590 IF P4=0 THEN R0=1
2600 FOR I=1 TO Nf
2610   Jm=0
2620   New=I+Nf
2630   FOR M=1 TO Model
2640     FOR J=1 TO Nterms
2650       IF Constant(M,J)=0 THEN 2750
2660       Jm=Jm+1
2670       Psave=P(M,J)
2680       P(M,J)=P(M,J)*1.1
2690       CALL Colem(I,1,"NO",Yfita,Yfitp,P(*),R(*))
2700       Dp=.1*Psave
2710       IF J=2 THEN Dp=.04139          !LGT TRANSFORM
2720       IF Iop<>2 THEN R(I,Jm)=LOG(Yfita/Yfit(1,I))/Dp
2730       IF Iop<>1 THEN R(New,Jm)=(FNAsnh(Yfitp)-FNAsnh(Yfit(1,New))
2740         )/Dp
2740       P(M,J)=Psave
2750     NEXT J
2760   NEXT M
2770   IF P4=0 THEN 2830
2780   Ro=R0
2790   R0=1.1*R0
2800   CALL Colem(I,1,"NO",Yfita,Yfitp,P(*),R(*))
2810   R(I,Jm+1)=LOG(Yfita/Yfit(1,I))*10/R0
2820   R0=R0
2830 NEXT I
2840 R0=R0
2850 RETURN
2860 Ro: Shift=0
2870   IF Iop=2 THEN Shift=Nf
2880   FOR I=1 TO Nf
2890     Fix=Yfit(1,I)
2900     IF P4=1 THEN Fix=1
2910     R0=Amp(1,I)/Fix
2920     IF Sigy(1,I+Shift)<>0 THEN 2940
2930   NEXT I
2940 RETURN
2950 Rchisqr: DIM Dy2(1,2*Nf)          !ERROR CALCULATION
2960           CALL Dy(Y(*),Yfit(*),Dy(*))
2970           MAT Dy2=Dy.Sigy
2980           MAT Dy2=Dy2.Dy2
2990           Chisq=SUM(Dy2)
3000           Rchisq=Chisq/Nfree
3010           RETURN
3020 End: Ans$="YES"
3030 PRINT "The reduced chi square has converged or diverged."
3040 PRINT "Type YES to plot your results. Type NO to change para
meters."
3050 INPUT "PLOT?",Ans$
3060 IF Ans$="NO" THEN Initialize
3070 SUBEND

```

```

3080 ! ****
3090 Dy!:! 11/81
3100 SUB Dy(SHORT Y(*),Yfit(*),Dy(*))
3110 !
3120 !    Y(*): Observed data
3130 !    Yfit(*): Calculated data
3140 !    Dy(*): Difference vector
3150 !
3160 OPTION BASE 1
3170 COM Nf,M,Pdev,Iop,Log$[3],Fnm$[6],Date$[8]
3180 COM SHORT R0,F(*),Amp(*),Phz(*),Constant(*)
3190 ON KEY #8 GOTO End
3200 DEF FNAshn(SHORT X)=LOG(X+SQR(X^2+1)) !ARC-HYPERBOLIC SINE
3210 Amp: IF Iop=2 THEN Phz
3220 FOR I=1 TO Nf
3230     Dy(1,I)=LOG(Y(1,I)/(R0*Yfit(1,I)))
3240 NEXT I
3250 Phz:IF (Iop=1) OR (Iop=4) THEN End
3260 FOR I=1 TO Nf
3270     Dy(1,I+Nf)=FNAshn(Y(1,I+Nf))-FNAshn(Yfit(1,I+Nf))
3280 NEXT I
3290 End:SUBEND
3300 ! ****
3310 Norm!:! NORMALIZATION 11/81
3320 SUB Norm(N,SHORT X(*),Y(*))
3330 !
3340 !    N: Dimensions of X and Y      NOTE: There may be problems
3350 !    X(*): Input array           if Xii gets 'close' to zero
3360 !    Y(*): Output array
3370 !
3380 OPTION BASE 1
3390 SHORT I(N,N),D(N,N)
3400 ON KEY #8 GOTO End
3410     MAT Y=(1)
3420     MAT I=IDN
3430     MAT D=(1)/X
3440     MAT D=I.D
3450     MAT I=D*Y
3460     MAT Y=I*D
3470     MAT Y=ABS(Y)
3480     MAT Y=SQR(Y)
3490     MAT Y=Y.X
3500 End: SUBEND

```

```

3510 ! ****
3520 Output!: INVERSION OUTPUT 11/81
3530 SUB Output(Form,Ix,Jx,K1,K2,K3,Tab1,SHORT X(*))
3540 !
3550 ! Form: format type
3560 ! Ix: first index limit
3570 ! Jx: second index limit
3580 ! K1: \
3590 ! K2: > constants
3600 ! K3: /
3610 ! Tab1: TAB argument
3620 ! X(*): output matrix (Ix,Jx)
3630 !
3640 OPTION BASE 1
3650 COM Nf,Mode1,Pdev,Iop,Log#[3],Fnm#[6],Date#[8]
3660 COM SHORT R0,F(*),Amp(*),Phz(*),Constant(*)
3670 DIM Header#[30],List#[94],Clist#[80],Col$(9)
3680 ON KEY #8 GOTO End
3690 DATA "M1 ","T1 ","C1 ","M2 ","T2 ","C2 ","M3 ","
T3 ","C3 "
3700 MAT READ Col$
3710 PRINTER IS Pdev,WIDTH(94)
3720 Ji=0
3730 FOR I=1 TO Ix
3740 IF Form=3 THEN Jx=I
3750 FOR J=1 TO Jx
3760 IF Form<>3 THEN 3790
3770 OUTPUT Plist$ USING "#,MD.DDD,4X";X(I,J)
3780 GOTO Sum
3790 IF (Form<>0) OR (Constant(I,J)<>0) THEN 3830
3800 OUTPUT Alist$ USING "#,X,4A,A";Col$((I-1)*3+J),":"
3810 OUTPUT Plist$ USING "#,MD.DDE,X";X(I,J)
3820 Clist$=Clist$&Alist$&Plist$
3830 IF Constant(I,J)=0 THEN 3890
3840 Ji=Ji+1
3850 IF Form=0 THEN OUTPUT Plist$ USING "#,4X,4A,4X";Col$((I-1)*
3+J)
3860 IF Form=1 THEN OUTPUT Plist$ USING "#,MD.DDE,X";X(I,J)
3870 IF Form=2 THEN OUTPUT Plist$ USING "#,MD.DDE,X";X(1,Ji)
3880 Sum: List$=List$&Plist$
3890 NEXT J
3900 IF Form=3 THEN PRINT TAB(Tab1);I;List$
3910 IF Form=3 THEN List$=""
3920 NEXT I
3930 IF Form=3 THEN End
3940 IF Form=2 THEN PRINT "%Sigma=";TAB(Tab1);List$
3950 IF Form=1 THEN OUTPUT Header$ USING "#,DE,2X,D.DDE,2X";K2,K3
3960 IF Form=1 THEN PRINT K1;TAB(Tab1);TRIM$(Header$&List$)
3970 IF Form=0 THEN PRINT "CONSTANT PARAMETERS:";TRIM$(Clist$)
3980 IF Form=0 THEN PRINT TRIM$("It Lamda Rchisq "&List$)
3990 End: PRINTER IS 16,WIDTH(80)
4000 SUBEND

```

```

4010 ! ****
4020 !
4030 Colem!! FORWARD AND DERIVATIVE COLE-COLE ALGORITHMS 11/81
4040 !
4050 ! ****
4060 !
4070 SUB Colem(I,It,Deriv$,SHORT Afit,Pfit,P(*),A(*))
4080 !
4090 ! I: current index from calling program
4100 ! It: seed for output files
4110 ! Deriv$: calculate analytic derivatives?, "YES" or "NO"
4120 ! Afit: best fit amplitude
4130 ! Pfit: best fit phase
4140 ! P(*): input parameter matrix (M,1)=M,(M,2)=T,(M,3)=C
4150 ! A(*): output derivative matrix (I,Model)
4160 !
4170 OPTION BASE 1
4180 COM Nf,Mm,Pdev,Iop,Log$[3],Fnm$[6],Date$[8]
4190 COM SHORT R0,F(*),Amp(*),Phz(*),Constant(*)
4200 SHORT C(0:1),Q(0:1),Z(0:Mm-1,2),Pd(0:Mm*3-1,2),Dadw(Mm)
4210 P2=PI/2
4220 Nterms=3
4230 C(0)=1
4240 C(1)=0
4250 IF (Log$="DBL") AND (Mm>>1) THEN Cup1$="YES"
4260 FOR M=1 TO Mm
4270     It=It+1
4280     N=M-1
4290     Sgn=-1
4300     IF (Cup1$="YES") AND (M=Mm) THEN Sgn=-Sgn
4310     W=2*PI*F(1,I)
4320     Wt=W*ABS(P(M,2))
4330     Wc=Wt^P(M,3)
4340     W2c=Wc^2
4350     A=Wc*COS(P2*P(M,3))
4360     B=Wc*SIN(P2*P(M,3))
4370     K1=A+W2c
4380     D1=1+2*A+W2c
4390     Re=Sgn*P(M,1)*K1/D1
4400     Z(N,1)=1+Re
4410     Im=Sgn*B*P(M,1)/D1
4420     Z(N,2)=Im
4430     !
4440     Amp(It,I)=Afit=R0*(Z(N,1)^2+Z(N,2)^2)^.5
4450     Phz(It,I)=Pfit=1000*ATN(Z(N,2)/Z(N,1)) !Phz in mrad's
4460     Cr=C(0)
4470     Ci=C(1)
4480     C(0)=Cr*Z(N,1)-Ci*Z(N,2) !COMPLEX PRODUCTS
4490     C(1)=Cr*Z(N,2)+Ci*Z(N,1)
4500     !
4510     IF Deriv$="NO" THEN 4630 !PARTIAL DIFFERENTIALS
4520     Inc=N*Nterms
4530     Kc=Sgn*P(M,1)/D1^2
4540     Kt=Kc*P(M,3)/P(M,2)

```

```

4550 Pd(Inc,1)=Sgn*K1/D1
4560 Pd(Inc,2)=Sgn*B/D1
4570 Ret=2*W2c+A*(1+W2c)
4580 Pd(1+Inc,1)=Kt*Ret
4590 Imt=B*(1-W2c)
4600 Pd(1+Inc,2)=Kt*Imt
4610 Pd(2+Inc,1)=Kc*(Ret*LOG(Wt)-P2*Imt)
4620 Pd(2+Inc,2)=Kc*(P2*Ret+Imt*LOG(Wt))
4630 NEXT M
4640 !                                     Amp AND Phz FOR
4650 Tan=C(1)/C(0)                         !TOTAL RELAXATION
4660 Rsave=C(0)
4670 IF Mm=1 THEN 4740
4680 Pextra=0
4690 IF C(0)<0 THEN Pextra=Sgn*3141.59      !SECOND&THIRD QUAD
4700 It=It+1
4710 Amp(It,I)=Afit=R0*(C(0)^2+C(1)^2)^.5
4720 Phz(It,I)=Pfit=1000*ATN(Tan)+Pextra
4730 !
4740 IF Deriv$="NO" THEN End
4750 D3=R0*SQR(1/(1+Tan^2))
4760 D4=1000/(Rsave*(1+Tan^2))
4770 D3=D3/Afit                         !Log TRANSFORM
4780 D4=D4/SQR(1+Pfit^2)                  !Asinh TRANSFORM
4790 New=I+Nf
4800 Jm=0
4810 FOR M=1 TO Mm                         !DERIVATIVES
4820   C(0)=1
4830   C(1)=0
4840 FOR K=1 TO Mm
4850   IF M=K THEN Skip
4860   Cr=C(0)
4870   Ci=C(1)
4880   C(0)=Cr*Z(K-1,1)-Ci*Z(K-1,2)      !PARTIAL PRODUCTS
4890   C(1)=Cr*Z(K-1,2)+Ci*Z(K-1,1)
4900 Skip: NEXT K
4910 FOR J=1 TO Nterms
4920   N=M-1
4930   Id=J-1+N*Nterms
4940   Q(0)=C(0)*Pd(Id,1)-C(1)*Pd(Id,2)  !PARTIAL DIFFERENTIAL
4950   Q(1)=C(0)*Pd(Id,2)+C(1)*Pd(Id,1)
4960   IF Constant(M,J)=0 THEN 5020
4970   Jm=Jm+1
4980   A(I,Jm)=D3*(Q(0)+Q(1)*Tan)
4990   IF J=2 THEN A(I,Jm)=2.3025*P(M,2)*A(I,Jm)
5000   A(New,Jm)=D4*(Q(1)-Q(0)*Tan)
5010   IF J=2 THEN A(New,Jm)=2.3025*P(M,2)*A(New,Jm)
5020 NEXT J
5030 NEXT M
5040 IF R0=1 THEN End
5050 A(I,Jm+1)=1/R0                      !ie. Afit/(R0*Afit)
5060 A(New,Jm+1)=0
5070 End: SUBEND

```

```

5080 ! ****
5090 !
5100 Weight!: DATA WEIGHTING 11/81
5110 !
5120 ! ****
5130 !
5140 SUB Weight(SHORT Y(*),Sigy(*),Ywt(*))
5150 !
5160 ! Y(*): input data vector (1,2*Nf)
5170 ! Sigy(*): standard deviation vector (1,2*Nf)
5180 ! Ywt(*): output weight vector (1,2*Nf)
5190 !
5200 OPTION BASE 1
5210 COM Nf,Model,Pdev,Iop,Log$[3],Fnm$[6],Date$[8]
5220 COM SHORT R0,F(*),Amp(*),Phz(*),Constant(*)
5230 DIM List$[123],Punc$[1],Comma$[1],Break$[1]
5240 MAT Ywt=(1)
5250 R0=Amp(1,1)
5260 Ans$="CONT"
5270 INPUT "Do you want to PLOT and preview the spectrum or CONT?
",Ans$
5280 IF Ans$="CONT" THEN Inv_op
5290 Preview: Model=0
5300 CALL Crplt(10,-3,5,"N",Ywt(*))
5310 CALL Argplt(Ywt(*))
5320 WAIT 3000
5330 EXIT GRAPHICS
5340 Inv_op: Iop=3
5350 PRINT ****
5360 PRINT " 1) Just Amplitude"
5370 PRINT " 2) Just Phase"
5380 PRINT " 3) Both Amp and Phz"
5390 PRINT ****
5400 INPUT "What do you want to invert?",Iop
5410 PRINT
5420 Wt_op: Wop=4
5430 PRINT ****
5440 PRINT " 1) Instrumental (1/sig^2)"
5450 PRINT " 2) Statistical (1/Y)"
5460 PRINT " 3) Selective (1-θ)"
5470 PRINT " 4) None (1)"
5480 PRINT ****
5490 INPUT "Choose one method of weighting the data?",Wop
5500 MAT Ywt=ZER
5510 PRINT PAGE
5520 Alist: IF Iop=2 THEN Plist
5530   Plist$="AMPLITUDE"
5540   Shift=0
5550   GOSUB Wt
5560 Plist: IF Iop=1 THEN End
5570   Plist$="PHASE"
5580   Shift=Nf
5590   GOSUB Wt

```

```

5600 GOTO End
5610 Wt: ON Wop GOTO Inst,Stat,Se1,None
5620 Inst: !
5630   FOR I=1 TO Nf
5640     IF Sigy=0 THEN Sigy=1
5650     Ywt(1,I+Shift)=1/Sigy^2
5660   NEXT I
5670 RETURN
5680 Stat: !
5690   FOR I=1 TO Nf
5700     Y=Y(1,I+Shift)
5710     IF Y=0 THEN Y=1
5720     Ywt(1,I+Shift)=1/ABS(Y)
5730   NEXT I
5740 RETURN
5750 Se1: !
5760   GOSUB List
5770   Comma$=","
5780   Break$="|"
5790   FOR I=1 TO Nf-1
5800   Ct=Ct+1
5810   Punc$=Comma$
5820   IF Ct=5 THEN Punc$=Break$
5830   IF Ct=5 THEN Ct=0
5840   OUTPUT Plist$ USING "#,3A";" "&"1"&Punc$
5850   List$=List$&Plist$
5860   NEXT I
5870   List$=List$&" 1 "
5880 EDIT "Edit the weighting function; then CONT.",List$
5890   FOR I=1 TO Nf
5900     Ywt(1,I+Shift)=VAL(List$[1,2])
5910     List$=List$[4]
5920   NEXT I
5930 RETURN
5940 None: !
5950   FOR I=1 TO Nf
5960     Ywt(1,I+Shift)=1
5970   NEXT I
5980 RETURN
5990 List: Ct=0
6000 PRINT LIN(1),Plist$,LIN(1)
6010   FOR I=1 TO Nf
6020   Ct=Ct+1
6030   OUTPUT Plist$ USING "#,2X,MD.DDE";Y(1,I+Shift)
6040   List$=List$&Plist$
6050   IF I=Nf THEN Print
6060   IF Ct<>5 THEN 6100
6070 Print: PRINT List$
6080   List$=""
6090   Ct=0
6100   NEXT I
6110 RETURN
6120 End: SUBEND

```

```

6130 Readin!: ****
6140 !
6150 Test!: FORWARD MODELED DATA I/O 11/81
6160 !
6170 ! ****
6180 !
6190 SUB Test(SHORT Y(*),Sigy(*),Ywt(*))
6200 !
6210 OPTION BASE 1
6220 COM Nf,Model,Pdev,Iop,Log$(3],Fnm$(6],Date$(8]
6230 COM SHORT R0,F(*),Amp(*),Phz(*),Constant(*)
6240 Device$":C" !REMOVABLE DISK
6250 Input: INPUT "TEST:Filename?",Fnm$
6260 ASSIGN #1 TO Fnm$&Device$
6270 I=0
6280 Readloop: ON END #1 GOTO Reform
6290     I=I+1
6300     READ #1;F(1,I),Amp(1,I),Phz(1,I)
6310     Nf=I
6320 GOTO Readloop
6330 Reform: FOR I=1 TO Nf
6340     Y(1,I)=Amp(1,I)
6350     Y(1,I+Nf)=Phz(1,I)
6360     NEXT I
6370 CALL Weight(Y(*),Sigy(*),Ywt(*))
6380 Io: PRINTER IS Pdev
6390 PRINT LIN(1),"FREQUENCY      AMP      WEIGHT      PHZ
WEIGHT"
6400 FOR I=1 TO Nf
6410     PRINT USING "D.DDE,2X,2(MD.DDE,3X,D.DD,3X)";F(1,I),Amp(1,I)
, Ywt(1,I),Phz(1,I),Ywt(1,I+Nf)
6420 NEXT I
6430 End: PRINTER IS 16
6440 SUBEND
6450 ! ****
6460 !
6470 ! USER SUPPLIED INPUT PROGRAMS
6480 !
6490 In1: SUB In1(SHORT Y(*),Sigy(*),Ywt(*))
6500 !
6510 In2: SUB In2(SHORT Y(*),Sigy(*),Ywt(*))
6520 !

```

```

6530 ! ****
6540 !
6550 Crplt!: PLOTS SPECTRAL IP DATA 11/81
6560 !
6570 ! ****
6580 !
6590 SUB Crplt(Base,Xmn,Xmx,Decup1$,SHORT Ywt(*))
6600 !
6610 ! Base: base system for frequency scale
6620 ! Xmn: minimum log10 frequency
6630 ! Xmx: maximum log10 frequency
6640 ! Decup1$: plot decoupled phase?(Y or N)
6650 ! Ywt(*): data weights (1,2*Nf)
6660 !
6670 OPTION BASE 1
6680 COM Nf,Model,Pdev,Iop,Log$[3],Fnm$[6],Date$[8]
6690 COM SHORT R0,F(*),Amp(*),Phz(*),Constant(*)
6700 SHORT X<1,Nf>,Z<Model+3,Nf>
6710 DIM Title$[40],Sym$(Nf)[1],Blank$(Nf)[1]
6720 P2=PI/2
6730 J1=2
6740 M=Model+2
6750 IF Model=0 THEN M=1
6760 IF Model=0 THEN J1=1
6770 IF Model=1 THEN M=2
6780 IF Decup1$="Y" THEN M=M+1
6790 FOR I=1 TO Nf
6800     X<1,I>=LOG(F<1,I>)/LOG(Base)
6810     Blank$(I)=""
6820     OUTPUT Sym$ USING "SD";-SGN(Phz<1,I>)
6830     Sym$(I)=Sym$[1,1]
6840     IF Ywt<1,I+Nf>=0 THEN Sym$(I)="#"
6850     FOR J=1 TO M
6860         Phz=-Phz<J,I>
6870         Z<J,I>=SGN(Phz)*LGT(ABS(Phz))
6880         IF (Phz>-1) AND (Phz<1) THEN Z<J,I>=0
6890     NEXT J
6900 NEXT I
6910 PLOTTER IS 13,"GRAPHICS"
6920 GRAPHICS
6930 LOCATE 5,118,20,99
6940 Phase: !
6950 Ymx=3
6960 Ymn=0
6970 Dely=1
6980 IF Log$="DBL" THEN Ymn=-3
6990 SCALE Xmn,Xmx,Ymn,Ymx
7000 AXES 1,ABS(Dely),Xmn,Ymn
7010 CALL Yax1b1(2,-P2,3.3,Ymn,Ymx,Dely,1,Xmn,.25,"LOG PHASE LAG (m
rad) .....")

```

```

7020 FOR J=J1 TO M
7030   CALL Linplt(Nf,3,1,J,Blank$(*),X(*),Z(*))
7040 NEXT J
7050   CALL Linplt(Nf,2,1,1,Sym$(*),X(*),Z(*))
7060 !
7070 Rk=1
7080 IF (Amp(M,1)>1.2) OR (Amp(M,1)<.2) THEN Rk=R0
7090 IF Decup1$="Y" THEN M=M-1
7100 FOR I=1 TO Nf
7110   Sym$(I)="0"
7120   IF Ywt(1,I)=0 THEN Sym$(I)="#"
7130   Z(M,I)=Amp(M,I)/Rk
7140   Z(1,I)=Amp(1,I)/R0
7150 NEXT I
7160 Amplitude: !
7170 Ymx=1
7180 Ymn=0
7190 Dely=.1
7200 SCALE Xmn,Xmx,Ymn,Ymx
7210 AXES 1,Dely,Xmx,Ymx
7220 CALL Yax1b1(8,-P2,3.3,Ymn,Ymx,Dely,1,Xmx,.25,"NORMALIZED AMPLITUDE -- - --")
7230   CALL Linplt(Nf,4,1,M,Blank$(*),X(*),Z(*))
7240   CALL Linplt(Nf,2,1,1,Sym$(*),X(*),Z(*))
7250 Labels: !
7260 CALL Xax1b1(6,0,3.3,Xmn,Xmx,1,1,Ymn,.05,"LOG10 FREQUENCY (Hz)")
)
7270 OUTPUT Title$ USING "7A,X,6A,XX,4A,D.DE";" FILE: ",Fnm$,"Rdc=",
,R0
7280 CALL Title((Xmx-Xmn)/2+Xmn,-.1,0,5,Title$)
7290 End: SUBEND

```

```

7300 ! ****
7310 !
7320 P1ots!:! PLOTTING SUBROUTINE PACKAGE 11/81
7330 !
7340 ! ****
7350 Rescale!:! RESCALES ARGAND AXIS TO LOOK GOOD
7360 SUB Rescale(Del,Mn,Mx)
7370 Sc=1/Del
7380 IF Mx>0 THEN Mx=(INT(Sc*Mx)+SGN(Mx))*Del
7390 IF Mx<0 THEN Mx=(INT(Sc*Mx)-SGN(Mx))*Del
7400 ! IF Mx=0 THEN Mx=Del
7410 IF Mn<0 THEN Mn=INT(Sc*Mn)*Del
7420 IF Mn>0 THEN Mn=(INT(Sc*Mn)-SGN(Mn))*Del
7430 ! IF Mn=0 THEN Mn=-Del
7440 SUBEND
7450 !
7460 ! **** LINE PLOT
7470 Linplt!:!
7480 SUB Linplt(Nf,Lintyp,Jx,Jy,Sym$(*),SHORT X(*),SHORT Y(*))
7490 !
7500 ! Nf: # of data points
7510 ! Lintyp: LINE TYPE argument
7520 ! Jx: constant index on X(*)
7530 ! Jy: constant index on Y(*)
7540 ! Sym$(*): plotting symbol (Nf)
7550 ! X(*): independent variable (Jx,Nf)
7560 ! Y(*): dependent variable (Jy,Nf)
7570 !
7580 LORG 5
7590 Ipen=-2
7600 FOR I=1 TO Nf
7610 LINE TYPE Lintyp
7620 PLOT X(Jx,I),Y(Jy,I),Ipen
7630 IF Sym$(I)="" THEN 7680
7640 WHERE X,Y
7650 LINE TYPE 1
7660 LABEL USING "K";Sym$(I)
7670 MOVE X,Y
7680 Ipen=-1
7690 IF I=Nf THEN 7710
7700 IF X(Jx,I)>X(Jx,I+1) THEN Ipen=-2
7710 NEXT I
7720 LINE TYPE 1
7730 End:SUBEND
7740 !
7750 ! ****
7760 !

```

```

7770 ! Lorg: LORG argument
7780 ! Ldir: LDIR argument
7790 ! Csize: CSIZE argument
7800 ! (X,Y)mn: minimum axis value
7810 ! (X,Y)mx: maximum axis value
7820 ! Del(x,y): axis STEP
7830 ! (X,Y)scale: multiplicative axis label scaling factor
7840 ! (Y,X): conjugate axis intersection
7850 ! (Y,X)shift: conjugate axis offset
7860 ! Label$: axis label
7870 !
7880 Xaxlbl!: X-AXIS LABEL
7890 SUB Xaxlbl(Lorg,Ldir,Csize,Xmn,Xmx,Delx,Xscale,Y,Yshift,Label$)
>
7900 CSIZE Csize
7910 LORG Lorg
7920 Isgn=1 !Lorg=4
7930 IF Lorg=6 THEN Isgn=-1 !Lorg=6
7940 FOR I=Xmn+Delx TO Xmx-Delx STEP Delx
7950 MOVE I,Y
7960 SETGU
7970 WHERE Xx,Yy
7980 MOVE Xx,Yy+Isgn*2.5
7990 SETUU
8000 LABEL USING "K";I*Xscale
8010 NEXT I
8020 LDIR Ldir
8030 LORG 5
8040 MOVE Xmnt+(Xmx-Xmn)/2,Y-Isgn*Yshift
8050 LABEL USING "K";Label$
8060 LDIR 0
8070 SUBEND
8080 !
8090 Yaxlbl!: Y-AXIS LABEL
8100 SUB Yaxlbl(Lorg,Ldir,Csize,Ymn,Ymx,Dely,Yscale,X,Xshift,Label$)
>
8110 CSIZE Csize
8120 LORG Lorg
8130 Isgn=1 !Lorg=2
8140 IF Lorg=8 THEN Isgn=-1 !Lorg=8
8150 FOR I=Ymn+Dely TO Ymx-Dely STEP Dely
8160 MOVE X,I
8170 II=I
8180 IF I=0 THEN II=1
8190 IF Lorg=2 THEN Yscale=SGN(I)*10^ABS(I)/II
8200 LABEL USING "X,K,X";I*Yscale
8210 NEXT I
8220 LDIR Ldir
8230 LORG 5
8240 CSIZE 3.3
8250 MOVE X-Isgn*Xshift,Ymn+(Ymx-Ymn)/2
8260 LABEL USING "K";Label$
8270 LDIR 0
8280 SUBEND

```

```
8290 !
8300 ! ****
8310 Title!:!                                     !PRINTS TITLE
8320 SUB Title(X,Y,Ldir,Csize,Label$)
8330 !
8340 !    X,Y: title position
8350 !    Ldir: LDIR argument
8360 !    Csize: CSIZE argument
8370 !    Label$: plot title
8380 !
8390 LORG 5
8400 LDIR Ldir
8410 CSIZE Csize
8420 MOVE X,Y
8430 LABEL USING "K";Label$
8440 CSIZE 3.3
8450 SUBEND
```

```

8460 ! ****
8470 !
8480 Argplt!: REAL AND IMAGINARY ARGAND PLOT           11/81
8490 !
8500 ! ****
8510 !
8520 SUB Argplt(SHORT Ywt())
8530 OPTION BASE 1
8540 COM Nf,M,Pdev,Iop,Log$[3],Fnm$[6],Date$[8]
8550 COM SHORT R0,F(*),A(*),P(*),Constant(*)
8560 SHORT Re(5,Nf),Im(5,Nf)
8570 ! Rmn=Imn=0                                     ! FORCES FULL NORMALIZED SCALE
8580 ! Rmx=Imx=0                                    ! REMOVE R, Iflag
8590 Rflag=Iflag=0
8600 FOR J=1 TO 1! M+1                         ! JUST PLOT OBSERVED DATA
8610 Rk=1
8620 IF (A(J,1)>1.2) OR (A(J,1)<.2) THEN Rk=R0
8630 FOR I=1 TO Nf
8640     Re(J,I)=A(J,I)/Rk*COS(P(J,I)/1000)
8650     IF (Iop>>2) AND (Ywt(1,I)=0) THEN 8710
8660     IF (Iop=2) AND (Ywt(1,I+Nf)=0) THEN 8710
8670     IF Rflag=0 THEN Rmn=Rmx=Re(J,I)
8680     Rflag=1
8690     Rmx=MAX(Rmx,Re(J,I))
8700     Rmn=MIN(Rmn,Re(J,I))
8710     Im(J,I)=A(J,I)/Rk*SIN(P(J,I)/1000)
8720     IF (Iop>>1) AND (Ywt(1,I+Nf)=0) THEN 8780
8730     IF (Iop=1) AND (Ywt(1,I)=0) THEN 8780
8740     IF Iflag=0 THEN Imn=Imx=Im(J,I)
8750     Iflag=1
8760     Imx=MAX(Imx,Im(J,I))
8770     Imn=MIN(Imn,Im(J,I))
8780 NEXT I
8790 NEXT J
8800 Delr=.1
8810 Deli=.1
8820 CALL Rescale(Delr,Rmn,Rmx)
8830 CALL Rescale(Deli,Imn,Imx)
8840 Nr=(Rmx-Rmn)/Delr
8850 Ni=(Imx-Imn)/Deli
8860 Nmx=MAX(Nr,Ni)
8870 IF Nr<>Nmx THEN Rmn=Rmn-INT((Nmx-Nr)/2)*Delr
8880 IF Ni<>Nmx THEN Imn=Imn-INT((Nmx-Ni)/2)*Deli
8890 Rmx=Rmn+Nmx*Delr
8900 Imx=Imn+Nmx*Deli

```

```

8910 PLOTTER 13 IS ON
8920 GRAPHICS
8930 LOCATE 19.1,45.43,20,46.33
8940 LORG 5
8950 SCALE Rmn,Rmx,Imx,Imn
8960 AXES Delr,Deli,Rmn,0
8970 CALL Xax1b1(6,0,3.3,INT(2*Rmn)/2,INT(2*Rmx)/2+.5,.5,1,0,0,"")
8980 CALL Yax1b1(8,-PI/2,3.3,INT(2*Imn)/2,INT(2*Imx)/2+.5,.5,1,Rmn
,0,"")
8990 FOR J=1 TO M+1
9000 Lintyp=3
9010 IF J=1 THEN Lintyp=1
9020 LINE TYPE Lintyp
9030 MOVE Re(J,1),Im(J,1)
9040 Ct=0
9050 FOR I=1 TO Nf
9060 Ct=Ct+1
9070 Ipen=-1
9080 IF J<>1 THEN 9190
9090 IF ((Iop<>2) AND (Ywt(1,I)=0) THEN 9120
9100 IF ((Iop=2) OR (Iop=3)) AND (Ywt(1,I+Nf)=0) THEN 9120
9110 PLOT Re(J,I),Im(J,I),Ipen
9120 WHERE X,Y
9130 IF (Ct<>4) OR (J<>1) THEN 9190
9140 LINE TYPE 1
9150 LABEL USING "K";"+"
9160 LINE TYPE Lintyp
9170 MOVE X,Y
9180 Ct=0
9190 NEXT I
9200 NEXT J
9210 SUBEND

```